Why not in process industries?

Challenges in Process Industries

Multiscale nature of process operations offers the main challenge

- **Pilot scale Experiments**
  - Lumped, homogeneous, input/output models
    - Equipment scale (ASPEN/HYSYS)
  - Process Performance

- **Lab Experiments**
  - Tray efficiency
  - overall heat/mass transfer
  - Volume averaged equations: Eulerian-Eulerian models
  - Time averaged equations: Turbulence models
  - Eulerian-Lagrangian models: Discrete Particle Models
  - Interpenetrating continuum scale (FLUENT/MFiX)

- **Stokesian Dynamics, Macro Particle Direct Numerical Simulation**
  - Navier-Stokes equation
  - Continuum scale (FLUENT/OpenFOAM/MFiX)

- **Lab Experiments**
  - Drage/lift forces
  - Interface heat/mass transfer

- **Lab Experiments**
  - Material Properties
    - viscosity, density, surface tension
    - **MD simulation**
      - Molecular scale (GROMACS)
  - Intermolecular Interaction potential

\[ \sum m_i = 0 \]

\[ \frac{Dv}{Dt} = -\nabla p + \rho g + \mu \nabla v^2 \]

\[ \frac{du}{dt} = \sum F \]